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QSPR study of the retention/release property of odorant molecules in pectin gels using statistical methods

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Abstract: *ACD/ChemSketch, MarvinSketch, and ChemOffice programs were used to calculate several molecular descriptors of 51 odorant molecules (15 alcohols, 11 aldehydes, 9 ketones and 16 esters). The best descriptors were selected to establish the quantitative structure property relationship (QSPR) of the retention/release property of odorant molecules property in pectin gels using principal components analysis (PCA), multiple linear regression (MLR), multiple non-linear regression (MNLR) and an artificial neural network (ANN) methods. We propose a quantitative model according to these analyses. The principal component analysis (PCA) has been used to select descriptors that show a high correlation with Property. The multiple linear regression (MLR) method showed a correlation coefficient of 0.960 and 0.958 for PG-0.4 (pectin concentration: 0.4% w/w) and PG-0.8 (pectin concentration: 0.8% w/w) medias, respectively. Internal and external validations were used to determine the statistical quality of QSPR of the two MLR models. The multiple non-linear regression (MNLR) method, considering the relevant descriptors obtained from the MLR, showed a correlation coefficient of 0.978 and 0.975 for PG-0.4 and PG-0.8 medias, respectively. The applicability domain of MLR models was investigated using simple and leverage approaches to detect outliers and outsides compounds. The effects of different descriptors in the property are described; and these descriptors were used to study and design of new compounds with higher and lower values property than the existing ones.*

Keywords: Odorant molecules, Retention/Release, Pectin gels, Quantitative Structure Property Relationship, Multiple Linear Regression, Artificial Neural Network.

1. INTRODUCTION

Pectin is a natural product which can be found in the cell walls of all higher plants and it has long been used for its gel formation, thickening and stabilising properties in a wide range of applications from food to the pharmaceutical and cosmetic industries. Pectin is a natural part of human diet, being present in fruits and vegetables, but does not contribute significantly to nutrition. Pectin passes through the small intestine more or less intact. Pectin is therefore a highly-sophisticated stabiliser recognised globally by consumers as label friendly and as one of the most important sources of dietary fibre.

Consumption of pectin has been shown to reduce blood cholesterol levels. The mechanism appears to be an increase of viscosity in the intestinal tract, leading to a reduced absorption of cholesterol from bile or food. In the large intestine and colon, microorganisms degrade pectin and liberate short-chain fatty acids that have a positive influence on health (prebiotic effect).

Odorant molecules, which are commonly known as aroma compounds, play a crucial role in the organoleptic quality of food and its acceptability by consumers [1]. Thus, the formulation of new fat-free food products (with pectin) requires an understanding of the physicochemical properties